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A Simple Relation between Percentage Ionic Character and Electronegativity Difference of Halides of Group 1 Elements.

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Abstract: *The percentage ionic character has been studied by several workers in the past. In this paper we have made an attempt to search a simple relation of percentage ionic character (PIC) and electronegativity difference of group 1 halides. The equation obtained is of the form PIC=m(x_A- x_B) + c. The values of m(Slope),c(Intercept) and r(correlation coefficient)have been found out. The trend of m and c has also been investigated.*

Keywords: *Percentage ionic character, Halides, Electronegativity difference,Intercept, Simple relation.*

I. Introduction

The percentage ionic character of Chemical bonds had been attracted by several researchers. The pioneers in this field were J.C. Phillips[1], C.H.Townes& B.P. Dailey[2]. E.S. Rittner[3], P.Kislink[4], Pauling[5], P.N.Schatz[6], M.J. Huggins[7], Hannay& Smith[8]. The methods of estimation of ionic character by the above researchers are difficult and time taking in computation. It has been observed that none of the methods give values which are in close agreement.In the present paper, it has been attempted to find a simple relation for estimation of percentage Ioniccharacter of halides of Group 1 elements.

II. Computation of Data

In the first phase, Pauling's is relation has been usedi.e. PIC=100[$1 - e^{\frac{-1}{4}(x_A - x_B)^2}$….(1)

for computing PIC of Chemical bonds with different elements,where, x_A- x_B=Electionegativity difference.The percentage ioniccharacter of halides of Group 1 elements have been estimated using the above equation and these values have been tabulated in table 1 to 4.

III. Simple Relation:

In the second phase, with the calculated values of percentage ionic character and electronegativity difference of the considered chemical bonds, we plotted graphs of PIC vs (x_A- x_B).It is found that the graphs are surprisingly straight lines, which gave a clue for setting up a linear and simple relationship between PIC and (x_A- x_B) of group I Elements. Since the plots of PIC vs(x_A- x_B)are linear hence the relation between them may be set down as -

PIC=**m** (x_A- x_B) +**c** ....(2)

where,

m=Slope

x_A- x_B=electronegativity difference

and **c**=intercept

The values of slopes, intercepts and correlation coefficient (r) have been found out by simple programming. The values of **m**, **c** and **r** have been mentioned in table 1 to 4 and collectively in table 5.It is clear from equation (2) that even if x_A- x_B= 0, the value of percentage ionic character of chemical bonds have some value which is equal to the value of intercept. We termed this value as Residual percentage ionic character of the chemical bond. It may be expected due to the structural features of the molecules.

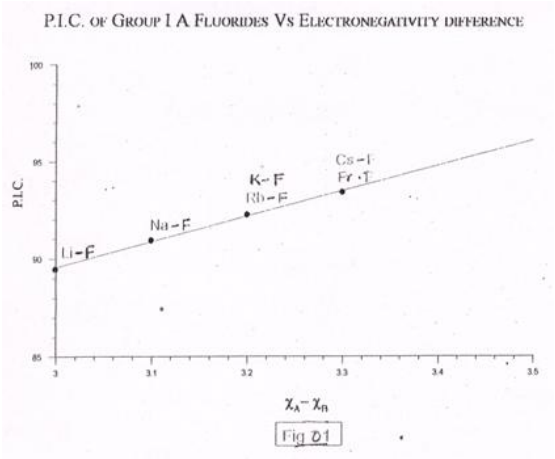
IV. Calculations of Percentage Ionic Character

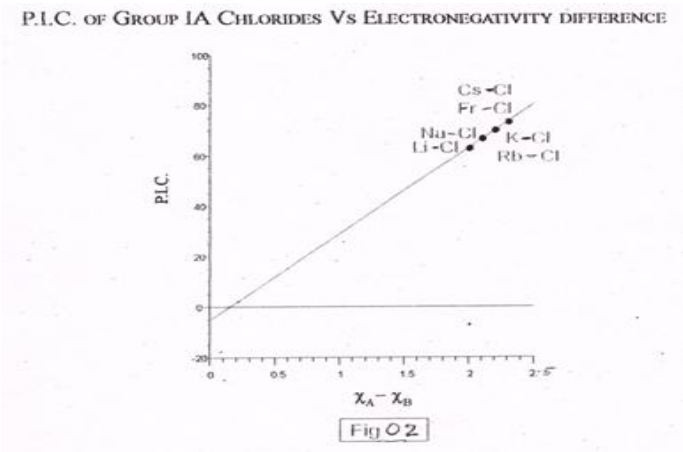
Table 1: P.I.C. Of Group I Fluorides

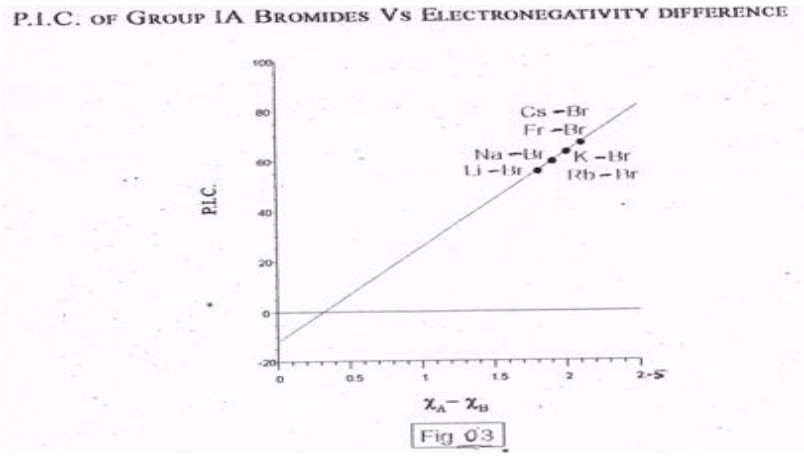
Bond	x_A- x_B	P.I.C. (Pauling)	P.I.C.=m(x_A- x_B) + c	Value of m, c, & r
Li-F	3	89.46	89.5630	
Na-F	3.1	90.95	90.8728	**m** = 13.09805
K-F	3.2	92.96	92.1826	**c**= 50.26888
Rb-F	3.2	92.96	92.1826	**r** = 0.9984
Cs-F	3.3	93.43	93.4924	
Fr-F	3.3	93.43	93.4924	

Table 2: P.I.C. Of Group I Chlorides

Bond	x_A- x_B	**P.I.C. (Pauling)**	**P.I.C.=m(x_A- x_B)**	**Value of m, c, & r**
Li-F	3	63	63.2010	
Na-F	2.1	66.79	66.6232	**m** = 34.22195
K-C1	2.2	70.18	70.0454	**c** =−5.24293
Rb-C1	2.2	70.18	70.0454	**r** = 0.9992
Cs-C1	2.3	73.35	73.4676	
Fr-C1	2.3	73.35	73.4676	







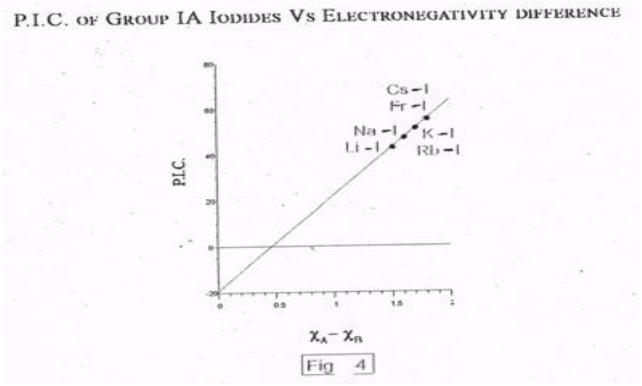


Fig 4

Table 3:P.I.C. Of Group I Bromides

Bound	$x_A - x_B$	**P.I.C. (Pauling)**	**P.I.C.=m($x_A - x_B$) + c**	**Value of m, c, & r**
Li-Br	1.8	55.51	55.6203	
Na-Br	1.9	59.44	59.3683	**m** = 37.48049
K- Br	2	63.21	63.1164	**c** = −11.84863
Rb- Br	2	63.21	63.1164	**r** = 0.9998
Cs- Br	2.1	66.79	63.8644	
Fr- Br	2.1	66.79	66.8644	

Table 4:P.I.C. Of Group I Iodides

Bound	$x_A - x_B$	**P.I.C. (Pauling)**	**X.=m($x_A - x_B$) + c**	**Value of m, c, & r**
Li-Br	1.5	43.02	43.0766	
Na-I	1.6	47.27	47.2339	**m**= 41.57317
K- I	1.7	51.44	51.3912	**c** = −19.328317
Rb- I	1.7	51.44	51.3912	**r** = 0.9999
Cs- I	1.8	55.51	55.5485	
Fr- I	1.8	55.51	55.5485	

Table 5:P.I.C. Of Group I Halides

PIC OF Group1 FLUORIDES	**m=13.09805**	**c =50.26888**	**r=0.9984**
PIC OF Group1 CHLORIDES	**m=34.22195**	**c =−5.24293**	**r=0.9992**
PIC OF Group1 BROMIDES	**m=37.48049**	**c =−11.84463**	**r=0.9998**
PIC OF Group1 IODIDES	**m=41.57317**	**c =−19.28317**	**r=0.9999**

V. Results & Discussion

We have computed the value of PIC of bonds with the help of equation (2)and found that the values are in close agreement with the value calculated from Pauling relation. One of the special feature of our equation is that it is simple one, less time taking in calculation and it uses only two constants **m**&**c** for estimation of percentage ionic character.

It is also clear from table 5 that the values of slope (m) varies from 13 to 41 for Group 1 halides. It is pertinent to note that the '**c**' values have been found to be negative quantity in almost all cases except in case of flurides of Group I. The negative value of '**c**' may indicate the residual covalency percentage of the chemical bond considered. The positive value of '**c**' incase of fluorides may indicate the Residual PIC of the bond considered.

From the table 5, it is worthwhile to note that there is an increasing trend of '**m**' incase of halides of Group I elements. No trend has been observed in case of '**c**' values. It is also observed from the tables that bonds between atoms with electronegativity difference 1.7 have 50 percent ionic character. Thus larger electronegativity difference in a bond result more ionic character. The bond between fluorine and any of the above considered elements are largely ionic in character. The sequence of ***ionicity*** in all groups are-

Fluoride>Chloride>Bromide>Iodide

It is also remarkable that bonds between fluorine and elements of Group I are maximum ionic in Character, for example Cs-F and Fr- F are 93 percentage ionic in Character.At the end, we can safely say that our proposed equation is superior to other equations with regard to its simplicity.

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